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Search Results
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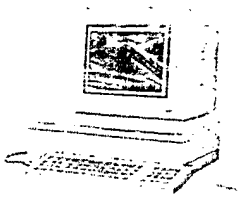

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The search results generated for your recent request are attached. If you have any questions or comments (compliments or complaints) about the scope or the results of the search, please contact ***the BioTech-Chem searcher*** who conducted the search ***or contact***:

Mary Hale, Supervisor, 308-4258
CM-1 Room 1E01

Voluntary Results Feedback Form

- *I am an examiner in Workgroup:* *(Example: 1610)*
- *Relevant prior art **found**, search results used as follows:*
  - ☐ 102 rejection
  - ☐ 103 rejection
  - ☐ Cited as being of interest.
  - ☐ Helped examiner better understand the invention.
  - ☐ Helped examiner better understand the state of the art in their technology.

Types of relevant prior art found:

- ☐ Foreign Patent(s)
- ☐ Non-Patent Literature
  (journal articles, conference proceedings, new product announcements etc.)

- *Relevant prior art **not found**:*
  - ☐ Results verified the lack of relevant prior art (helped determine patentability).
  - ☐ Search results were not useful in determining patentability or understanding the invention.

Other Comments:

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DICTIONARY FILE UPDATES:  12 FEB 2003  HIGHEST RN 489395-53-1

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  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

Crossover limits have been increased.  See HELP CROSSOVER for details.

Experimental and calculated property data are now available.  See HELP
PROPERTIES for more information.  See STNote 27, Searching Properties
in the CAS Registry File, for complete details:
http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

=> d sta que 19
L1              STR
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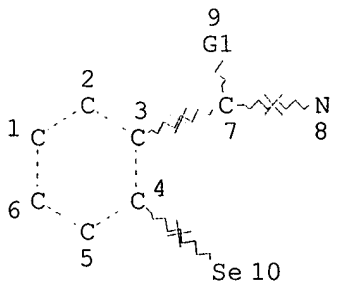


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L7              STR
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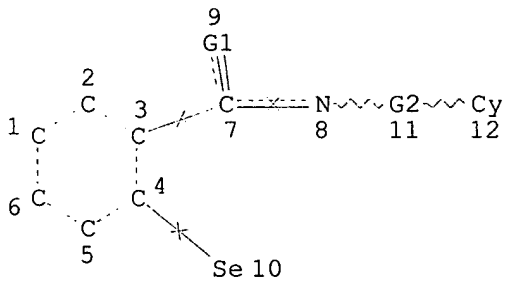

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STEREO ATTRIBUTES: NONE
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100.0% PROCESSED    726 ITERATIONS                          461 ANSWERS
SEARCH TIME: 00.00.01


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L3                STR L1
L4             40 S L3
L5            726 S L1 FUL
                  SAV L5 KUMAR926/A
L6                STR L1
L7                STR L6
L8             17 S L7 SAM SUB=L5
L9            461 S L7 FUL SUB=L5
                  SAV L9 KUMAR926A/A
L10               STR L7
L11             4 S L10 SAM SUB=L9
L12            69 S L10 FUL SUB=L9
                  SAV L12 KUMAR926B/A
L13               STR L10
L14           197 S L9 AND NSEC3-C6/ES
L15             2 S L9 AND NSEC3-OCOC2-C6/ES
L16           262 S L9 NOT L14,L15
L17           195 S L16 NOT L12
L18               STR L13
L19             6 S L9 AND OCOC2-C6/ES
L20           266 S L12,L14,L15
L21           195 S L9 NOT L20
L22               STR L18
L23            13 S L22 CSS SAM SUB=L9
L24           254 S L22 CSS FUL SUB=L9
                  SAV L24 KUMAR926C/A
L25            66 S L24 AND L12
L26             3 S L12 NOT L25
L27             2 S L26 NOT C28H20N2O6SE2
L28           254 S L24 AND L16
L29             8 S L16 NOT L28
L30             1 S L29 AND C21H17NO3SE
L31             4 S L19 NOT (C15H13NO3SE OR C14H9NO4SE)
L32            26 S L28 AND METHYLSELENO
L33           228 S L28 NOT L32
L34            85 S L33 AND S/ELS
L35            15 S L34 AND SULFONYL
L36            70 S L34 NOT L35
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L38          16 S L37 NOT C18H18N2O4SSE
L39          52 S L36 NOT L37
L40         143 S L33 NOT L34-L39

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                E HOLMGREN A/AU
L42         288 S E3-E5,E13
                E AMIRI M/AU
L43           7 S E3,E8,E10
                E MASAYASU H/AU
L44          33 S E3,E4
L45           2 S L41 AND L42-L44
                E DAIICHI/PA,CS
                E DAIICH/PA,CS
L46        8279 S E3-E18
                E DAICH/PA,CS
L47          22 S E13,E14
L48           7 S L41 AND L46,L47
L49           8 S L45,L48
L50           8 S L5 AND L49

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L51           1 S 139015-80-8
L52           1 S 60940-34-3
L53           1 S 9074-14-0

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L54         696 S L53
L55        1104 S THIOREDOXIN REDUCTASE OR (NADP OR NADPH)(S)THIOREDOXIN(S)REDU
L56        1117 S L54,L55
L57         518 S L5
L58           7 S L56 AND L57
L59         112 S L42-L47 AND L56
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L61          14 S L50,L58,L60
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L66           3 S L65 NOT E1-E6
L67          12 S L64,L66
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L68          31 S E7-E37
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L80 8 S L78,L79

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FILE COVERS 1907 - 13 Feb 2003 VOL 138 ISS 7
FILE LAST UPDATED: 12 Feb 2003 (20030212/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d l80 all hitstr tot

L80 ANSWER 1 OF 8 HCAPLUS COPYRIGHT 2003 ACS
AN 2002:783160 HCAPLUS
TI A Novel Antioxidant Mechanism of Ebselen Involving Ebselen Diselenide, a Substrate of Mammalian Thioredoxin and **Thioredoxin Reductase**
AU Zhao, Rong; Holmgren, Arne
CS Department of Medical Biochemistry and Biophysics, Medical Nobel Institute for Biochemistry, Karolinska Institutet, Stockholm, SE-171 77, Swed.
SO Journal of Biological Chemistry (2002), 277(42), 39456-39462
CODEN: JBCHA3; ISSN: 0021-9258
PB American Society for Biochemistry and Molecular Biology
DT Journal
LA English
CC 7-3 (Enzymes)
Section cross-reference(s): 6
AB The antioxidant mechanism of ebselen involves recently discovered redns. by mammalian **thioredoxin reductase** (TrxR) and thioredoxin (Trx) forming ebselen selenol. Here we describe a previously unknown reaction; ebselen reacts with its selenol forming an ebselen diselenide with a rate const. of 372 M-1s-1. The diselenide also was a substrate of TrxR forming the selenol with Km of 40 .mu.M and kcat of 79 min-1 (kcat/Km of 3.3 .times. 104 M-1s-1). Trx increased the redn. because of its fast reaction with diselenide (rate const. 1.7 .times. 103 M-1s-1). Diselenide stimulated the H2O2 reductase activity of TrxR, even more efficiently with Trx present. Because the mechanism of ebselen as an antioxidant has been assumed to involve glutathione peroxidase-like activity, we compared the H2O2 reductase activity of ebselen with the GSH and Trx systems. TrxR at 50 nM, far below the estd. physiol. level, gave 8-fold higher activity compared with 1 mM GSH; addn. of 5 .mu.M Trx increased this difference to 13-fold. The rate const. of ebselen selenol reacting with H2O2 was estd. to be faster than 350 M-1s-1. We propose

novel mechanisms for ebselen antioxidant action involving ebselen selenol and diselenide formation, with the thioredoxin system rather than glutathione as the predominant effector and target.

ST ebselen antioxidant diselenide thioredoxin peroxide reductase

IT INDEXING IN PROGRESS

IT Antioxidants
Enzyme kinetics
Michaelis constant
(novel ebselen antioxidant action involves ebselen selenol and diselenide formation with thioredoxin system as predominant effector and target)

IT Thioredoxins
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(novel ebselen antioxidant action involves ebselen selenol and diselenide formation with thioredoxin system as predominant effector and target)

IT **9074-14-0, Thioredoxin reductase**
60940-34-3, Ebselen
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(novel ebselen antioxidant action involves ebselen selenol and diselenide formation with thioredoxin system as predominant effector and target)

RE.CNT 53 THERE ARE 53 CITED REFERENCES AVAILABLE FOR THIS RECORD

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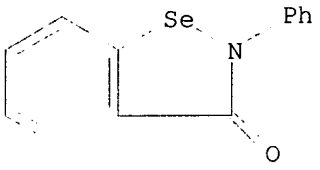
IT INDEXING IN PROGRESS

IT **9074-14-0, Thioredoxin reductase**
60940-34-3, Ebselen
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(novel ebselen antioxidant action involves ebselen selenol and diselenide formation with thioredoxin system as predominant effector and target)

RN 9074-14-0 HCAPLUS
CN Reductase, thioredoxin (9CI) (CA INDEX NAME)

RN 60940-34-3 HCAPLUS
CN 1,2-Benzisoselenazol-3(2H)-one, 2-phenyl- (9CI) (CA INDEX NAME)



L80 ANSWER 2 OF 8 HCAPLUS COPYRIGHT 2003 ACS
AN 2002:519211 HCAPLUS
DN 138:83310
TI Ebselen: a substrate for human **thioredoxin reductase** strongly stimulating its hydroperoxide reductase activity and a superfast thioredoxin oxidant
AU Zhao, Rong; Masayasu, Hiroyuki; Holmgren, Arne
CS Medical Nobel Institute for Biochemistry, Department of Medical Biochemistry and Biophysics, Karolinska Institute, Stockholm, SE-171 77, Swed.
SO Proceedings of the National Academy of Sciences of the United States of America (2002), 99(13), 8579-8584
CODEN: PNASA6; ISSN: 0027-8424
PB National Academy of Sciences
DT Journal
LA English
CC 1-12 (Pharmacology)
AB Ebselen [2-phenyl-1,2-benzisoselenazol-3(2H)-one], a seleno-org. compd. with glutathione peroxidase-like activity is used in clin. trials against stroke. Human and bovine TrxR catalyzed the redn. of ebselen to ebselen selenol by NADPH with an apparent KM-value of 2.5 .mu.M and a kcat of 588 min-1. The addn. of thioredoxin (Trx) stimulated the TrxR-catalyzed redn. of ebselen several-fold. This result was caused by a very fast oxidn. of reduced Trx by ebselen with a rate const. in excess of 2.times.107 M-1 s-1. This rate is orders of magnitude faster than the reaction of dithiol

Trx with insulin disulfides. Ebselen competed with disulfide substrates for redn. by Trx and, therefore, acted as an inhibitor of protein disulfide redn. by the Trx system. The inherent H2O2 reductase activity of mammalian TrxR dependent on its active-site selenocysteine residue was stimulated 10-fold by 2 .mu.M ebselen and 25-fold in the addnl. presence of 5 .mu.M Trx. Furthermore, the apparent KM-value of TrxR for H2O2 was lowered 25-fold to about 100 .mu.M. Our results demonstrate that ebselen is a TrxR peroxidase which, in the presence of Trx, acted as a mimic of a peroxiredoxin. The activity with TrxR and oxidn. of reduced Trx offer mechanistic explanations for the in vivo effects of ebselen as an antioxidant and anti-inflammatory agent. Our results demonstrate that the mechanism of action of ebselen may be predominantly via the Trx system rather than via glutathione.

ST ebselen **thioredoxin reductase** hydroperoxide antioxidant human **NADPH**

IT Anti-inflammatory agents
Antioxidants
Human
(ebselen is a substrate for human **thioredoxin reductase** strongly stimulating its hydroperoxide reductase activity and a superfast thioredoxin oxidant)

IT Brain, disease
(stroke; ebselen is a substrate for human **thioredoxin reductase** strongly stimulating its hydroperoxide reductase activity and a superfast thioredoxin oxidant)

IT 53-57-6, **NADPH** 9013-66-5, Glutathione peroxidase **9074-14-0, Thioredoxin reductase**
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(ebselen is a substrate for human **thioredoxin reductase** strongly stimulating its hydroperoxide **reductase** activity and a superfast **thioredoxin** oxidant)

IT **60940-34-3**, Ebselen
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(ebselen is a substrate for human **thioredoxin reductase** strongly stimulating its hydroperoxide reductase activity and a superfast thioredoxin oxidant)

RE.CNT 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

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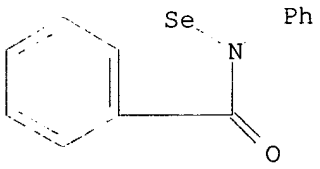
IT **9074-14-0, Thioredoxin reductase**
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(ebselen is a substrate for human **thioredoxin reductase** strongly stimulating its hydroperoxide reductase activity and a superfast thioredoxin oxidant)
RN 9074-14-0 HCAPLUS
CN Reductase, thioredoxin (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
IT **60940-34-3**, Ebselen
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(ebselen is a substrate for human **thioredoxin reductase** strongly stimulating its hydroperoxide reductase activity and a superfast thioredoxin oxidant)
RN 60940-34-3 HCAPLUS
CN 1,2-Benzisoselenazol-3(2H)-one, 2-phenyl- (9CI) (CA INDEX NAME)



L80 ANSWER 3 OF 8 HCAPLUS COPYRIGHT 2003 ACS
AN 2001:669761 HCAPLUS
DN 136:35047
TI The biochemistry of selenium and the glutathione system
AU Arteel, G. E.; Sies, H.
CS Department of Pharmacology, Laboratory of Hepatobiology and Toxicology, University of North Carolina at Chapel Hill, Chapel Hill, NC, 27599-7365, USA
SO Environmental Toxicology and Pharmacology (2001), 10(4), 153-158
CODEN: ETOPFR; ISSN: 1382-6689
PB Elsevier Science B.V.
DT Journal; General Review
LA English
CC 13-0 (Mammalian Biochemistry)
Section cross-reference(s): 1
AB A review. In the context of defense against pro-oxidants, selenium and the glutathione (GSH) system play key functions. Major roles of GSH include direct interception of pro-oxidants, as well as a redn. of other

antioxidants from their oxidized forms. Furthermore, GSH has ancillary functions, such as metab., cell signaling, and protein interactions, that can also mediate defense against oxidants. Protection by selenium in the mammalian cell is mediated by selenol-amino acids, either as selenocystine or selenomethionine. The active site of the potent glutathione peroxidases (GPx) contains selenocystine residues. Furthermore, other selenoproteins (e.g. selenoprotein P and **thioredoxin reductase**) also have been shown to possess antioxidant properties. Synthetic organoselenium compds. (e.g. ebselen) have also shown promise as pharmacol. antioxidants in in vivo models of tissue damage due to oxidative stress. The specific function of selenoproteins and organoselenium compds. in defense against peroxynitrite, by redn. of this potent oxidizing and nitrating species to nitrite, is also discussed.

ST review selenium glutathione peroxynitrite oxidative stress antioxidant; ebselen antioxidant glutathione peroxidase selenoprotein oxidative stress review

IT Antioxidants
(biochem. of selenium and glutathione system)

IT Antioxidants
Oxidative stress, biological
(biochem. of selenium and glutathione system in relation to)

IT Proteins
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(selenium-contg.; biochem. of selenium and glutathione system)

IT 70-18-8, Glutathione, biological studies 7782-49-2, Selenium, biological studies 9013-66-5, Glutathione peroxidase
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(biochem. of selenium and glutathione system)

IT 19059-14-4, Peroxynitrite
RL: ADV (Adverse effect, including toxicity); BIOL (Biological study)
(biochem. of selenium and glutathione system in relation to)

IT **60940-34-3**, Ebselen
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(biochem. of selenium and glutathione system in relation to)

RE.CNT 66 THERE ARE 66 CITED REFERENCES AVAILABLE FOR THIS RECORD

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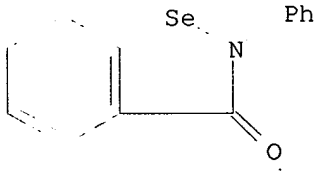
IT **60940-34-3**, Ebselen
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(biochem. of selenium and glutathione system in relation to)

RN 60940-34-3 HCAPLUS

CN 1,2-Benzisoselenazol-3(2H)-one, 2-phenyl- (9CI) (CA INDEX NAME)



L80 ANSWER 4 OF 8 HCAPLUS COPYRIGHT 2003 ACS

AN 2000:707140 HCAPLUS

DN 133:271642

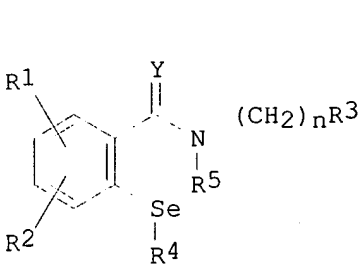
TI Use of 2-phenyl-1,2-benzisoselenazol-3(2H)-one or its derivatives as substrates for **thioredoxin reductase**

IN **Holmgren, Arne; Amiri, Marjan H.; Masayasu,**

Hiroyuki
PA Daiichi Pharmaceutical Co., Ltd., Japan
SO PCT Int. Appl., 34 pp.
CODEN: PIXXD2
DT Patent
LA Japanese
IC ICM C07C391-02
ICS A61K031-166; A61P039-06; B01J031-12; C07B031-00; C09K015-32; C12N009-00; C12N009-04
CC 63-5 (Pharmaceuticals)
Section cross-reference(s): 1, 7
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2000058281	A1	20001005	WO 2000-JP2076	20000331
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
EP 1174423	A1	20020123	EP 2000-913022	20000331
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				

PRAI JP 1999-92789 A 19990331
JP 1999-101478 A 19990408
WO 2000-JP2076 W 20000331
OS MARPAT 133:271642
GI



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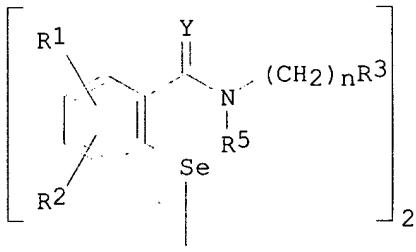

II

AB Substrates for **thioredoxin reductase**, contg. compds. represented by general formula (I) or (II) (such as 2-phenyl-1,2-benzisoselenazol-3(2H)-one (III) or open-ring derivs. thereof) (wherein R1 and R2 are each hydrogen, halogeno, trifluoromethyl, NO2, C1-6 alkyl or alkoxy; or R1 and R3 are combined together represent methylenedioxy; R3 is (un)substituted aryl, arom. heterocyclic group, or 5- to 7-membered cycloalkyl or cycloalkenyl; R4 is hydrogen, hydroxyl, an -S-.alpha.-amino acid group, or aralkyl optionally having 1 or .gtoreq.2 substituents; R5 is hydrogen or C1-6 alkyl; Y is oxygen or sulfur; and n is an integer of 0 to 5, with the proviso that the selenium atom may be oxidized) are described. These substrates are reduced by **thioredoxin reductase** in the presence of **NADPH** and enhance the peroxidase activity of **thioredoxin reductase**. A tablet formulation contg. III 50, CM-cellulose 25, starch 5, cryst. cellulose 40, and magnesium stearate 2 mg was prepd.
ST phenylbenzisoselenazolone substrate **thioredoxin**

reductase; peroxidase activity enhancement **thioredoxin reductase**

IT **139015-80-8**
RL: ANT (Analyte); BSU (Biological study, unclassified); MFM (Metabolic formation); PEP (Physical, engineering or chemical process); ANST (Analytical study); BIOL (Biological study); FORM (Formation, nonpreparative); PROC (Process)
(substrates for **thioredoxin reductase**)

IT **60940-34-3**, 2-Phenyl-1,2-benzisoselenazol-3(2H)-one
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PEP (Physical, engineering or chemical process); THU (Therapeutic use); BIOL (Biological study); PROC (Process); USES (Uses)
(substrates for **thioredoxin reductase**)

IT **9074-14-0, Thioredoxin reductase**
RL: BPR (Biological process); BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study); PROC (Process)
(substrates for **thioredoxin reductase**)

RE.CNT 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

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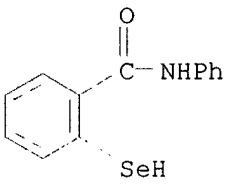
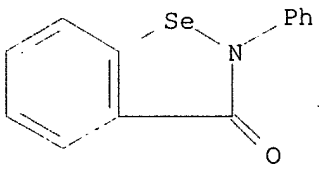
IT **139015-80-8**
RL: ANT (Analyte); BSU (Biological study, unclassified); MFM (Metabolic formation); PEP (Physical, engineering or chemical process); ANST (Analytical study); BIOL (Biological study); FORM (Formation, nonpreparative); PROC (Process)
(substrates for **thioredoxin reductase**)

RN 139015-80-8 HCAPLUS
CN Benzamide, N-phenyl-2-selenyl- (9CI) (CA INDEX NAME)



IT **60940-34-3**, 2-Phenyl-1,2-benzisoselenazol-3(2H)-one
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PEP (Physical, engineering or chemical process); THU (Therapeutic use); BIOL (Biological study); PROC (Process); USES (Uses)
(substrates for **thioredoxin reductase**)

RN 60940-34-3 HCAPLUS
CN 1,2-Benzisoselenazol-3(2H)-one, 2-phenyl- (9CI) (CA INDEX NAME)



IT **9074-14-0, Thioredoxin reductase**

RL: BPR (Biological process); BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study); PROC (Process)
(substrates for **thioredoxin reductase**)
RN 9074-14-0 HCAPLUS
CN Reductase, thioredoxin (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

L80 ANSWER 5 OF 8 HCAPLUS COPYRIGHT 2003 ACS
AN 2000:531379 HCAPLUS
DN 133:306449
TI Interaction of peroxynitrite with selenoproteins and glutathione peroxidase mimics
AU Sies, H.; Arteel, G. E.
CS Institut fur Physiologische Chemie I, Heinrich-Heine-Universitat Dusseldorf, Dusseldorf, Germany
SO Free Radical Biology & Medicine (2000), 28(10), 1451-1455
CODEN: FRBMEH; ISSN: 0891-5849
PB Elsevier Science Inc.
DT Journal
LA English
CC 4-3 (Toxicology)
Section cross-reference(s): 10
AB Peroxynitrite is an oxidant generated under inflammatory conditions, acting in defense against invading microorganisms. There is a need for protection of the organism from damage inflicted by peroxynitrite. Selenium-contg. compds., notably Ebselen, have a high second-order reaction rate const. (.apprx.2 .times. 106 M-1 s-1), which makes them candidates for efficient protection. This applies also for selenium in proteins, occurring as selenocysteine or selenomethionine residues. Glutathione peroxidases, **thioredoxin reductase**, and selenoprotein P have been shown to play a potential role in protection against peroxynitrite. Tellurium-contg. compds. also react with peroxynitrite.
ST peroxynitrite interaction selenoprotein glutathione peroxidase
IT Oxidative stress, biological
(interaction of peroxynitrite with selenoproteins and glutathione peroxidase mimics)
IT Radicals, biological studies
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); BIOL (Biological study); RACT (Reactant or reagent)
(interaction of peroxynitrite with selenoproteins and glutathione peroxidase mimics)
IT Proteins, specific or class
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); BIOL (Biological study); RACT (Reactant or reagent)
(selenium-contg., P; interaction of peroxynitrite with selenoproteins and glutathione peroxidase mimics)
IT Proteins, specific or class
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); BIOL (Biological study); RACT (Reactant or reagent)
(selenium-contg.; interaction of peroxynitrite with selenoproteins and glutathione peroxidase mimics)
IT 19059-14-4, Peroxynitrite
RL: ADV (Adverse effect, including toxicity); RCT (Reactant); BIOL (Biological study); RACT (Reactant or reagent)
(interaction of peroxynitrite with selenoproteins and glutathione peroxidase mimics)
IT 1464-42-2, Selenomethionine 3614-08-2, Selenocysteine 9013-66-5, Glutathione peroxidase **9074-14-0**, **Thioredoxin**

reductase 13494-80-9D, Tellurium, org. compds., biological studies **60940-34-3**, Ebselen
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); BIOL (Biological study); RACT (Reactant or reagent)
(interaction of peroxynitrite with selenoproteins and glutathione peroxidase mimics)

RE.CNT 47 THERE ARE 47 CITED REFERENCES AVAILABLE FOR THIS RECORD

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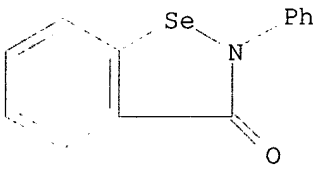
IT **9074-14-0, Thioredoxin reductase**
60940-34-3, Ebselen
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); BIOL (Biological study); RACT (Reactant or reagent)
(interaction of peroxynitrite with selenoproteins and glutathione peroxidase mimics)

RN 9074-14-0 HCAPLUS
CN Reductase, thioredoxin (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
RN 60940-34-3 HCAPLUS
CN 1,2-Benzisoselenazol-3(2H)-one, 2-phenyl- (9CI) (CA INDEX NAME)



L80 ANSWER 6 OF 8 HCAPLUS COPYRIGHT 2003 ACS
AN 1999:117100 HCAPLUS
DN 130:308314
TI Function of **Thioredoxin Reductase** as a Peroxynitrite Reductase Using Selenocystine or Ebselen
AU Arteel, Gavin E.; Briviba, Karlis; Sies, Helmut
CS Institut fuer Physiologische Chemie I, Heinrich-Heine-Universitaet Duesseldorf, Duesseldorf, D-40001, Germany
SO Chemical Research in Toxicology (1999), 12(3), 264-269
CODEN: CRTOEC; ISSN: 0893-228X
PB American Chemical Society
DT Journal
LA English
CC 7-3 (Enzymes)
Section cross-reference(s): 4
AB The activity of mammalian **thioredoxin reductase** as a peroxynitrite reductase was investigated. Peroxynitrite was infused to maintain a 0.2 .mu.M steady-state concn. in potassium phosphate buffer (pH 7.4). Benzoate hydroxylation and nitrite formation were used as indexes of oxidn. reactions of peroxynitrite and of peroxynitrite redn., resp. In the presence of **NADPH** (10 .mu.M), **thioredoxin reductase** at 50 nM alone did not significantly scavenge peroxynitrite, as shown by there being no significant effect on benzoate hydroxylation or nitrite formation. However, when selenocystine (1 .mu.M) or ebselen (2 .mu.M) was present in the reaction mixt., there was significant suppression of benzoate hydroxylation and an increase in nitrite formation until all the NADPH was oxidized. The addn. of thioredoxin did not enhance these effects. In contrast, peroxynitrite redn. by ebselen complexed with BSA was enhanced by the presence of thioredoxin. In parallel expts., **thioredoxin reductase** efficiently reduced ebselen selenoxide back to ebselen.
ST **thioredoxin reductase** peroxynitrite redn selenocystine ebselen
IT Thioredoxins
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(function of **thioredoxin reductase** as a peroxynitrite reductase using selenocystine or ebselen)
IT Albumins, biological studies
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(serum, ebselen complexes; function of **thioredoxin reductase** as a peroxynitrite reductase using selenocystine or ebselen)
IT **9074-14-0, Thioredoxin Reductase**
60940-34-3D, Ebselen, complexes with bovine serum albumin

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(function of **thioredoxin reductase** as a peroxynitrite reductase using selenocystine or ebselen)

IT 53-57-6, **Nadph** 19059-14-4, Peroxynitrite 29621-88-3, L-Selenocystine **60940-34-3**, Ebselen 104473-83-8, Ebselen selenoxide
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(function of **thioredoxin reductase** as a peroxynitrite **reductase** using selenocystine or ebselen)

RE.CNT 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

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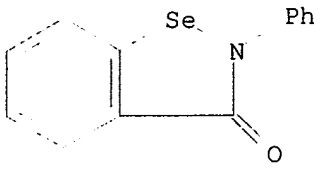
(28) Wagner, G; Biochem Pharmacol 1994, V48, P1137 HCAPLUS
(29) Yasuda, K; Biochem Biophys Res Commun 1980, V96, P243 HCAPLUS
(30) Zhong, L; J Biol Chem 1998, V273, P8581 MEDLINE

IT **9074-14-0**, **Thioredoxin Reductase**
60940-34-3D, Ebselen, complexes with bovine serum albumin
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(function of **thioredoxin reductase** as a peroxynitrite reductase using selenocystine or ebselen)

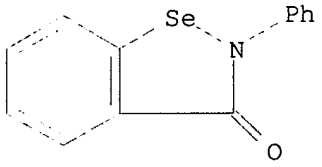
RN 9074-14-0 HCAPLUS
CN Reductase, thioredoxin (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 60940-34-3 HCAPLUS
CN 1,2-Benzisoselenazol-3(2H)-one, 2-phenyl- (9CI) (CA INDEX NAME)



IT **60940-34-3**, Ebselen
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(function of **thioredoxin reductase** as a peroxynitrite **reductase** using selenocystine or ebselen)
RN 60940-34-3 HCAPLUS
CN 1,2-Benzisoselenazol-3(2H)-one, 2-phenyl- (9CI) (CA INDEX NAME)



L80 ANSWER 7 OF 8 HCAPLUS COPYRIGHT 2003 ACS
AN 1998:200706 HCAPLUS
DN 128:265859
TI Diaryl chalcogenides as selective inhibitors of **thioredoxin reductase** and potential antitumor agents
AU Engman, Lars; Cotgreave, Ian; Angulo, Miguel; Taylor, Charles W.; Paine-Murrieta, Gillian D.; Powis, Garth
CS Department of Organic Chemistry, Institute of Chemistry, Uppsala University, Uppsala, 75121, Swed.
SO Anticancer Research (1997), 17(6D), 4599-4605
CODEN: ANTRD4; ISSN: 0250-7005
PB Anticancer Research
DT Journal
LA English
CC 1-6 (Pharmacology)
AB **Thioredoxin reductase** is a selenocysteine contg. flavoenzyme that catalyzes the **NADPH** dependent redn. of the redox protein **thioredoxin**. Thioredoxin is over-expressed by a no. of human tumors. Exptl. studies have shown that thioredoxin is responsible for the growth and transformed phenotype of some human cancer cells. Thus, **thioredoxin reductase** presents an attractive target for anticancer drug development to regulate the activity of the thioredoxin system. We have examd. a series of 12 organoselenium compds. and 16 organotellurium compds., mostly of the diaryl chalcogenide type, as inhibitors of human **thioredoxin reductase** and have investigated the cytotoxicity and antitumor activity of some of the compds. The organoselenium compd. Ebselen was found to be a competitive inhibitor of human **thioredoxin reductase** (Ki 2.8 .mu.M), while a no. of organotellurium compds. were found to be noncompetitive inhibitors (Kis 2.3 to 35.2 .mu.M). Human glutathione reductase was not appreciably inhibited by any of the compds., except for one dinitro organotellurium compd. that caused inhibition with an IC50 of 0.5 .mu.M and an over 20-fold selectivity compared to **thioredoxin reductase**. The compds. inhibited the growth of human cancer cells in culture with IC50s as low as 2 .mu.M Some organotellurium compds. when administered daily by i.p. injection to mice caused up to 50% inhibition

of the growth of MCF-7 human breast cancer xenografts but the relative insoly. of the compds. was a limiting factor in their use.

ST diaryl chalcogenide **thioredoxin reductase** antitumor

IT Antitumor agents
(diaryl chalcogenides as selective inhibitors of **thioredoxin reductase** and potential antitumor agents)

IT 149902-64-7P 205675-82-7P
RL: ADV (Adverse effect, including toxicity); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(diaryl chalcogenides as selective inhibitors of **thioredoxin reductase** and potential antitumor agents)

IT 35050-01-2 59130-74-4 **60940-34-3** 63212-74-8 65130-25-8 67516-66-9 77422-94-7 87345-08-2 96636-40-7 96748-33-3 104755-32-0 117402-62-7 135085-11-9 144381-99-7 144382-00-3 144382-01-4 144693-22-1 **144842-35-3** 152943-38-9 152943-49-2 155228-86-7 155228-87-8 155228-88-9 204519-52-8 205675-80-5 205675-81-6
RL: ADV (Adverse effect, including toxicity); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(diaryl chalcogenides as selective inhibitors of **thioredoxin reductase** and potential antitumor agents)

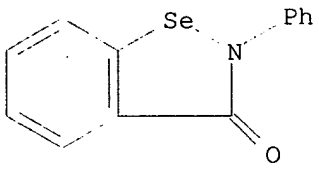
IT 9001-48-3, Glutathione reductase
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(diaryl chalcogenides as selective inhibitors of **thioredoxin reductase** and potential antitumor agents)

IT 110-02-1, Thiophene 112-89-0, Octadecyl bromide 77422-85-6 102945-08-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(diaryl chalcogenides as selective inhibitors of **thioredoxin reductase** and potential antitumor agents)

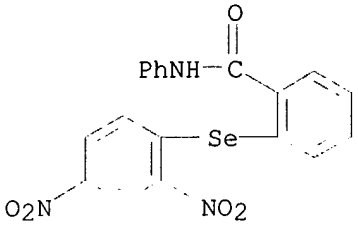
IT **9074-14-0, Thioredoxin reductase**
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(inhibitors; diaryl chalcogenides as selective inhibitors of **thioredoxin reductase** and potential antitumor agents)

IT **60940-34-3 144842-35-3**
RL: ADV (Adverse effect, including toxicity); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(diaryl chalcogenides as selective inhibitors of **thioredoxin reductase** and potential antitumor agents)

RN 60940-34-3 HCAPLUS
CN 1,2-Benzisoselenazol-3(2H)-one, 2-phenyl- (9CI) (CA INDEX NAME)



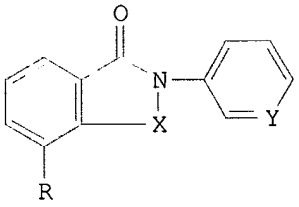
RN 144842-35-3 HCAPLUS
CN Benzamide, 2-[(2,4-dinitrophenyl)seleno]-N-phenyl- (9CI) (CA INDEX NAME)



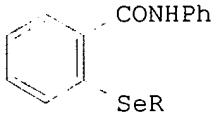
IT **9074-14-0, Thioredoxin reductase**
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(inhibitors; diaryl chalcogenides as selective inhibitors of **thioredoxin reductase** and potential antitumor agents)
RN 9074-14-0 HCAPLUS
CN Reductase, thioredoxin (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

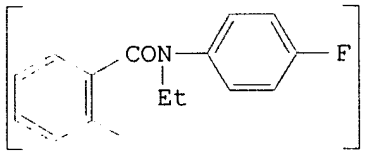
L80 ANSWER 8 OF 8 HCAPLUS COPYRIGHT 2003 ACS
AN 1990:565101 HCAPLUS
DN 113:165101
TI Mechanism for the inhibitory effect of a seleno-organic compound, ebselen, and its analogs on superoxide anion production in guinea pig polymorphonuclear leukocytes
AU Wakamura, Kyoko; Ohtsuka, Toshiaki; Okamura, Naoki; Ishibashi, Sadahiko; **Masayasu, Hiroyuki**
CS Sch. Med., Hiroshima Univ., Hiroshima, 734, Japan
SO Journal of Pharmacobio-Dynamics (1990), 13(7), 421-5
CODEN: JOPHDQ; ISSN: 0386-846X
DT Journal
LA English
CC 1-7 (Pharmacology)
GI



I, R=H, X=Se, Y=CH
II, R=H, X=S, Y=CH
III, R=NO_2, X=Se, Y=CH
IV, R=H, X=Se, Y=N



V, R=Me
VI, R=S(CO_2Na)$CHCH_2CO_2H$



VII

AB Effects of ebselen (I) and its analogs (PZ-25 (II), NAT06-123 (III), NAT02-761 (IV), NAT02-801 (V), NAT06-099 (VI), and NAT06-513 (VII)) on superoxide anion (O2-) prodn. induced by tetradecanoyl phorbol acetate (TPA) were examd. in intact guinea pig polymorphonuclear leukocytes (PMNL). Four compds. having a structure of 1,2 benzoisoselenazol-3-(2H)one (I, III, IV) and its sulfur-substituted analog (II), had a potent inhibitory effect on O2- prodn. as compared with others. I and III also markedly inhibited NADP (NADPH) oxidase activity, which is responsible for O2- prodn. in intact cells, and in a particulate fraction prepd. from TPA-stimulated PMNL, whereas II inhibited this enzyme weakly and I did not. On the other hand, I and II had the same degree of potent inhibitory effect on protein kinase C which was involved in the regulation of NADPH oxidase activation. Thus, it is plausible that inhibition of O2- prodn. in intact PMNL by these compds. were due not only to direct inhibition of NADPH oxidase but also to inhibition of protein kinase C.

ST ebselen superoxide formation inhibition polymorphonuclear leukocyte

IT Inflammation inhibitors
(ebselen and analogs as)

IT Leukocyte
(polymorphonuclear, superoxide formation by, ebselen and analogs inhibition of)

IT 9026-43-1, Protein kinase
RL: BIOL (Biological study)
(C, in polymorphonuclear leukocytes, ebselen and analogs effect on)

IT 7782-44-7D, Oxygen, radicals 11062-77-4, Superoxide
RL: FORM (Formation, nonpreparative)
(formation of, by polymorphonuclear leukocytes, ebselen and analogs inhibition of)

IT 9032-22-8, NADPH oxidase
RL: BIOL (Biological study)
(in polymorphonuclear leukocytes, ebselen and analogs effect on)

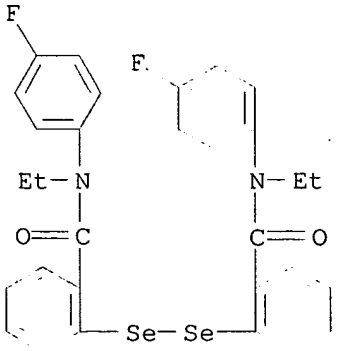
IT 2527-03-9, PZ 25 60940-24-1, NAT 06-099 60940-34-3, Ebselen 89780-24-5, NAT 06-123 **118528-47-5**, NAT 02-801 119214-92-5, NAT 02-761 **129836-90-4**, NAT 06-513
RL: BIOL (Biological study)
(superoxide formation by polymorphonuclear leukocytes inhibition by)

IT 7782-49-2D, Selenium, org. compds.
RL: BIOL (Biological study)
(superoxide formation by polymorphonuclear leukocytes inhibition by ebselen and analogs as)

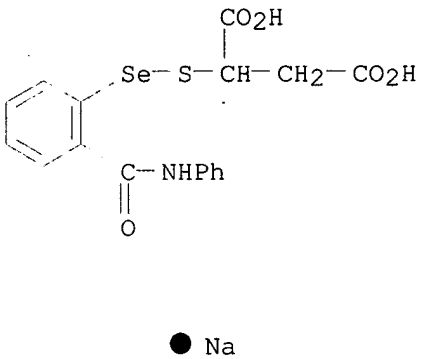
IT **118528-47-5**, NAT 02-801 **129836-90-4**, NAT 06-513
RL: BIOL (Biological study)
(superoxide formation by polymorphonuclear leukocytes inhibition by)

RN 118528-47-5 HCAPLUS

CN Benzamide, 2,2'-diselenobis[N-ethyl-N-(4-fluorophenyl)- (9CI) (CA INDEX NAME)



RN 129836-90-4 HCAPLUS
CN Butanedioic acid, [[[2-[(phenylamino)carbonyl]phenyl]seleno]thio]-, monosodium salt (9CI) (CA INDEX NAME)



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L83         136 S L56
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L85          43 S L81,L82
L86          35 S L85 AND A61K/IC,ICM,ICS
L87          34 S L85 AND (424 OR 514)/NCLM,NCLS
L88           8 S L85 NOT L86,L87
L89           4 S L88 NOT (SILVER OR GRIP OR DISKS)/TI
L90          39 S L86,L87,L89
L91          38 S L90 AND (PD<=20000331 OR PRD<=20000331 OR AD<=20000331)

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L93         495 S L92
L94           0 S L93 AND L74
L95           0 S L93 AND L9
L96          19 S L93 AND L5
L97           2 S L96 AND C22H21NOSE

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L98           1 S L97

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CA INDEXING COPYRIGHT (C) 2003 AMERICAN CHEMICAL SOCIETY (ACS)

FILE 'USPAT2' ENTERED AT 19:18:04 ON 13 FEB 2003
CA INDEXING COPYRIGHT (C) 2003 AMERICAN CHEMICAL SOCIETY (ACS)

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L98 ANSWER 1 OF 1 USPATFULL
AN 92:70344 USPATFULL
TI Anti-inflammatory benzylselenobenzamides made from anilines and benzylamines
IN Evers, Michel, Liege, Belgium
Fischer, Hartmut, Cologne, Germany, Federal Republic of
Biedermann, Jurgen, Pulheim, Germany, Federal Republic of
Terlinden, Rolf, Cologne, Germany, Federal Republic of
Leyck, Sigurd, Pulheim, Germany, Federal Republic of
PA A. Nattermann & Cie. GmbH, Cologne, Germany, Federal Republic of (non-U.S. corporation)
PI US 5141955 19920825
AI US 1990-611272 19901108 (7)
PRAI DE 1989-3937169 19891108
DT Utility
FS Granted
EXNAM Primary Examiner: Daus, Donald G.
LREP Dubno, Herbert
CLMN Number of Claims: 5
ECL Exemplary Claim: 1
DRWN No Drawings
LN.CNT 621
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
AB Anti-inflammatory benzylselanobenzamides made from anilines and benzylamines have the formula I ##STR1## are disclosed wherein R is hydrogen, methyl or ethyl;

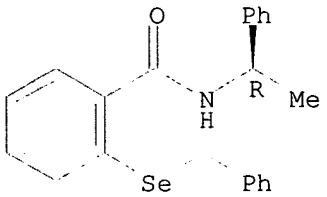
R.sup.1 and R.sup.2 are the same or different and, taken separately, are hydrogen, fluorine, chlorine, bromine, C.sub.1 to C.sub.4 alkyl, C.sub.1 to C.sub.4 alkoxy, hydroxy, cyano, amino, dimethylamino or nitro; and

R.sup.3 and R.sup.4 are the same or different and, taken separately, are hydrogen, fluorine, chlorine, bromine, C.sub.1 to C.sub.4 alkyl, C.sub.1 to C.sub.4 alkoxy, hydroxy, cyano, or nitro and, taken together, represent methylenedioxy; and

n is 0.1 or 2.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.
IT **135963-72-3P 135963-73-4P**
(prepn. of, as antiinflammatory)
RN 135963-72-3 USPATFULL
CN Benzamide, N-(1-phenylethyl)-2-[(phenylmethyl)seleno]-, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 135963-73-4 USPATFULL
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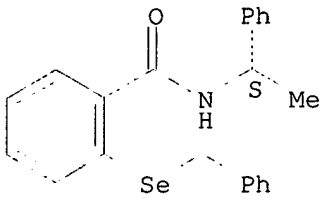
Absolute stereochemistry.



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L7 STR L6
L8 17 S L7 SAM SUB=L5
L9 461 S L7 FUL SUB=L5
SAV L9 KUMAR926A/A
L10 STR L7
L11 4 S L10 SAM SUB=L9
L12 69 S L10 FUL SUB=L9
SAV L12 KUMAR926B/A
L13 STR L10
L14 197 S L9 AND NSEC3-C6/ES
L15 2 S L9 AND NSEC3-OCOC2-C6/ES
L16 262 S L9 NOT L14,L15
L17 195 S L16 NOT L12
L18 STR L13
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L20 266 S L12,L14,L15
L21 195 S L9 NOT L20
L22 STR L18
L23 13 S L22 CSS SAM SUB=L9
L24 254 S L22 CSS FUL SUB=L9
SAV L24 KUMAR926C/A
L25 66 S L24 AND L12
L26 3 S L12 NOT L25
L27 2 S L26 NOT C28H20N2O6SE2
L28 254 S L24 AND L16
L29 8 S L16 NOT L28
L30 1 S L29 AND C21H17NO3SE
L31 4 S L19 NOT (C15H13NO3SE OR C14H9NO4SE)
L32 26 S L28 AND METHYLSELENO
L33 228 S L28 NOT L32
L34 85 S L33 AND S/ELS
L35 15 S L34 AND SULFONYL
L36 70 S L34 NOT L35
L37 18 S L36 AND GLYCINE
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                 E AMIRI M/AU
L43            7 S E3,E8,E10
                 E MASAYASU H/AU
L44           33 S E3,E4
L45            2 S L41 AND L42-L44
                 E DAIICHI/PA,CS
                 E DAIICH/PA,CS
L46         8279 S E3-E18
                 E DAICH/PA,CS
L47           22 S E13,E14
L48            7 S L41 AND L46,L47
L49            8 S L45,L48
L50            8 S L5 AND L49

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L53            1 S 9074-14-0

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L56         1117 S L54,L55
L57          518 S L5
L58            7 S L56 AND L57
L59          112 S L42-L47 AND L56
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L61           14 S L50,L58,L60
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                 SEL HIT RN

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L83         136 S L56
L84           0 S L81,L82 AND L83
L85          43 S L81,L82
L86          35 S L85 AND A61K/IC,ICM,ICS
L87          34 S L85 AND (424 OR 514)/NCLM,NCLS
L88           8 S L85 NOT L86,L87
L89           4 S L88 NOT (SILVER OR GRIP OR DISKS)/TI
L90          39 S L86,L87,L89
L91          38 S L90 AND (PD<=20000331 OR PRD<=20000331 OR AD<=20000331)

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     FILE 'REGISTRY' ENTERED AT 19:15:44 ON 13 FEB 2003
L93         495 S L92
L94           0 S L93 AND L74
L95           0 S L93 AND L9
L96          19 S L93 AND L5
L97           2 S L96 AND C22H21NOSE

     FILE 'USPATFULL, USPAT2' ENTERED AT 19:17:48 ON 13 FEB 2003
L98           1 S L97

     FILE 'USPATFULL, USPAT2' ENTERED AT 19:18:04 ON 13 FEB 2003

=> fil reg
FILE 'REGISTRY' ENTERED AT 19:18:18 ON 13 FEB 2003
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
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Property values tagged with IC are from the ZIC/VINITI data file
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STRUCTURE FILE UPDATES:   12 FEB 2003  HIGHEST RN 489395-53-1
DICTIONARY FILE UPDATES:  12 FEB 2003  HIGHEST RN 489395-53-1

TSCA INFORMATION NOW CURRENT THROUGH MAY 20, 2002

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

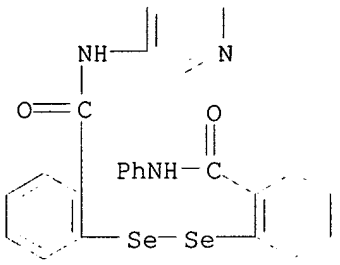
Crossover limits have been increased.  See HELP CROSSOVER for details.

Experimental and calculated property data are now available.  See HELP
PROPERTIES for more information.  See STNote 27, Searching Properties
in the CAS Registry File, for complete details:
http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

=> d scan l25

L25  66 ANSWERS   REGISTRY  COPYRIGHT 2003 ACS
IN   Benzamide, 2-[[2-[(phenylamino)carbonyl]phenyl]diseleno]-N-3-pyridinyl-
```

(9CI)
MF C25 H19 N3 O2 Se2

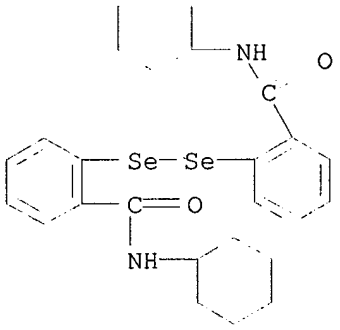


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):5

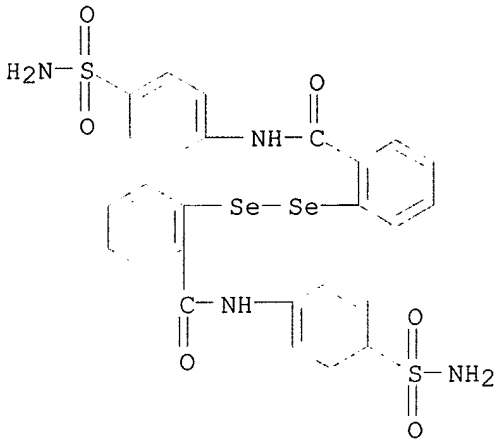
L25 66 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Benzamide, 2,2'-diselenobis[N-cyclohexyl- (9CI)
MF C26 H32 N2 O2 Se2

From here to end "free" view of sample cmpds



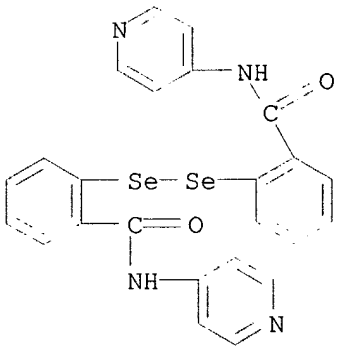
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L25 66 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Benzamide, 2,2'-diselenobis[N-[4-(aminosulfonyl)phenyl]- (9CI)
MF C26 H22 N4 O6 S2 Se2



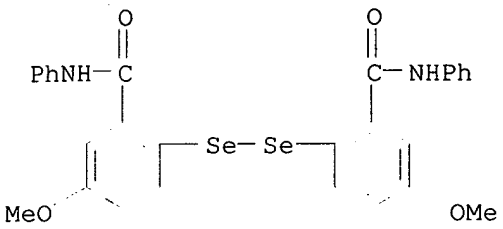
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L25 66 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Benzamide, 2,2'-diselenobis[N-4-pyridinyl- (9CI)
MF C24 H18 N4 O2 Se2



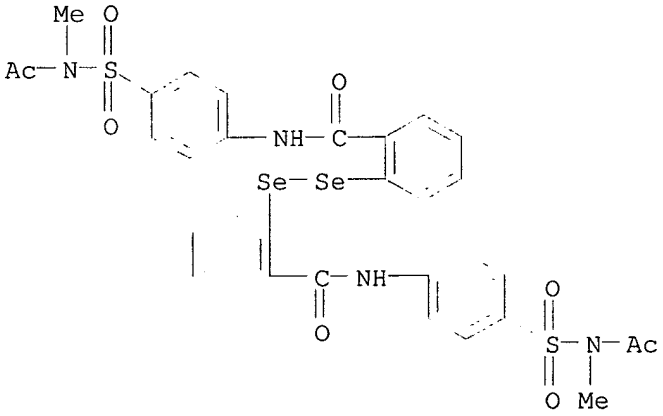
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L25 66 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Benzamide, 2,2'-diselenobis[5-methoxy-N-phenyl- (9CI)
MF C28 H24 N2 O4 Se2



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L25 66 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Benzamide, 2,2'-diselenobis[N-[4-[(acetylmethylamino)sulfonyl]phenyl]- (9CI)
MF C32 H30 N4 O8 S2 Se2



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

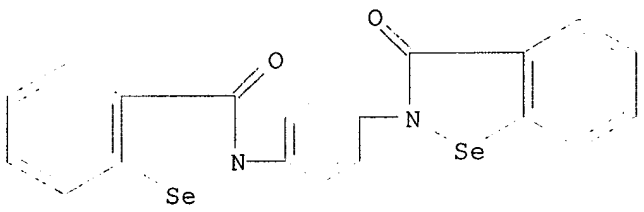
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):end

=> d sca l27

L27 2 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN 1,2-Benzisoselenazol-3(2H)-one, 2,2'-[1,1'-biphenyl]-4,4'-diylbis- (9CI)
MF C26 H16 N2 O2 Se2

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):

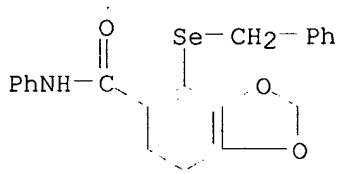
L27 2 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN 1,2-Benzisoselenazol-3(2H)-one, 2,2'-(1,4-phenylene)bis- (9CI)
MF C20 H12 N2 O2 Se2



ALL ANSWERS HAVE BEEN SCANNED

=> d sca l30

L30 1 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN 1,3-Benzodioxole-5-carboxamide, N-phenyl-4-[(phenylmethyl)seleno]- (9CI)
MF **C21 H17 N O3 Se**

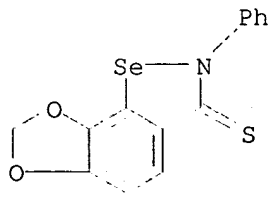


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

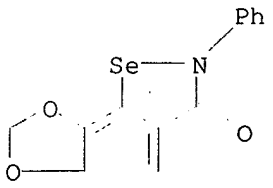
=> d scan l15

L15 2 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN [1,3]Dioxolo[4,5-g]-1,2-benzisoselenazole-3(2H)-thione, 2-phenyl- (9CI)
MF C14 H9 N O2 S Se



HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):

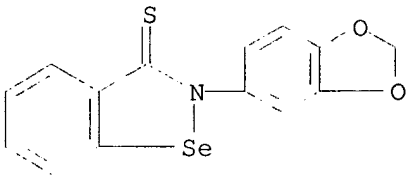
L15 2 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN [1,3]Dioxolo[4,5-g]-1,2-benzisoselenazol-3(2H)-one, 2-phenyl- (9CI)
MF C14 H9 N O3 Se



ALL ANSWERS HAVE BEEN SCANNED

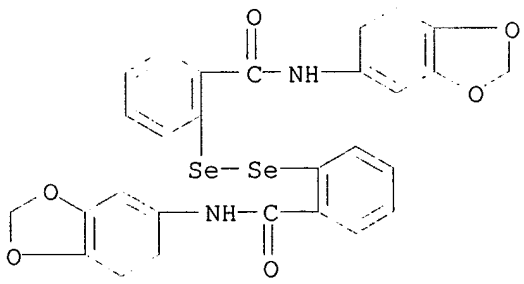
=> d sca l31

L31 4 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN 1,2-Benzisoselenazole-3(2H)-thione, 2-(1,3-benzodioxol-5-yl)- (9CI)
MF C14 H9 N O2 S Se



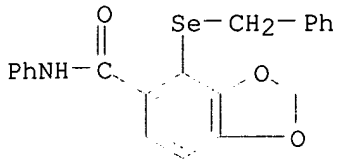
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):4

L31 4 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Benzamide, 2,2'-diselenobis[N-1,3-benzodioxol-5-yl- (9CI)
MF C28 H20 N2 O6 Se2



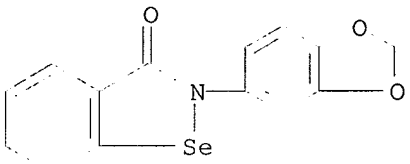
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L31 4 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN 1,3-Benzodioxole-5-carboxamide, N-phenyl-4-[(phenylmethyl)seleno]- (9CI)
MF C21 H17 N O3 Se



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

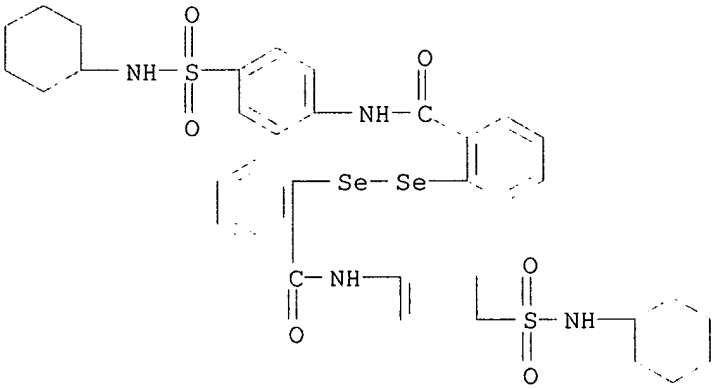
L31 4 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN 1,2-Benzisoselenazol-3(2H)-one, 2-(1,3-benzodioxol-5-yl)- (9CI)
MF C14 H9 N O3 Se



ALL ANSWERS HAVE BEEN SCANNED

=> d sca l35

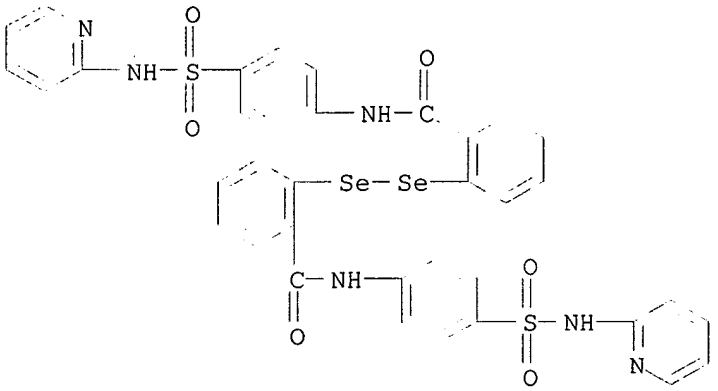
L35 15 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN **Benzamide, 2,2'-diselenobis[N-[4-[(cyclohexylamino)sulfonyl]phenyl]-(9CI)**
MF **C38 H42 N4 O6 S2 Se2**



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

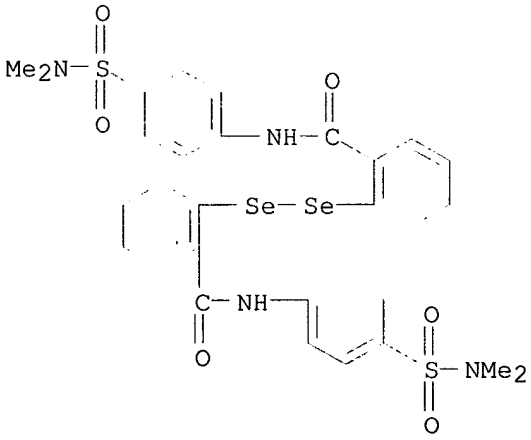
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):5

L35 15 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN **Benzamide, 2,2'-diselenobis[N-[4-[(2-pyridinylamino)sulfonyl]phenyl]-(9CI)**
MF **C36 H28 N6 O6 S2 Se2**



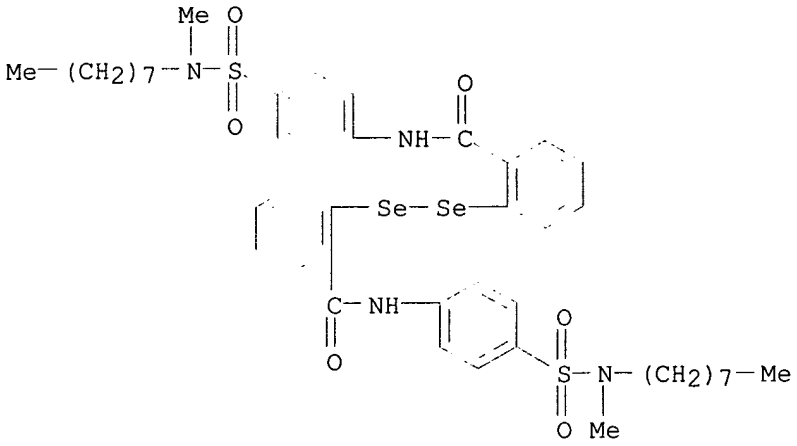
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L35 15 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN **Benzamide, 2,2'-diselenobis[N-[4-[(dimethylamino)sulfonyl]phenyl]-(9CI)**
MF **C30 H30 N4 O6 S2 Se2**



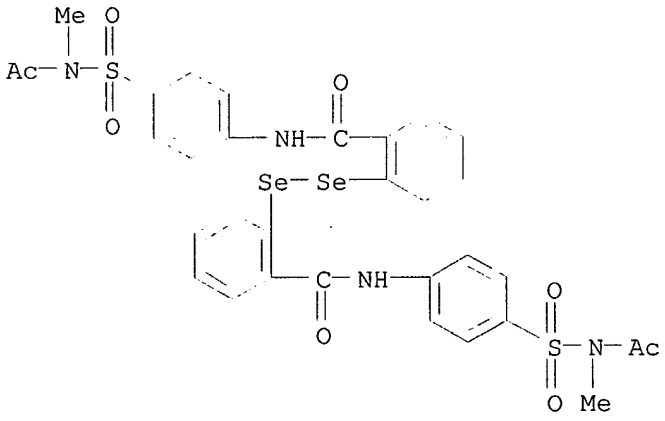
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L35 15 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN **Benzamide, 2,2'-diselenobis[N-[4-[(methyloctylamino)sulfonyl]phenyl]-(9CI)**
MF **C44 H58 N4 O6 S2 Se2**



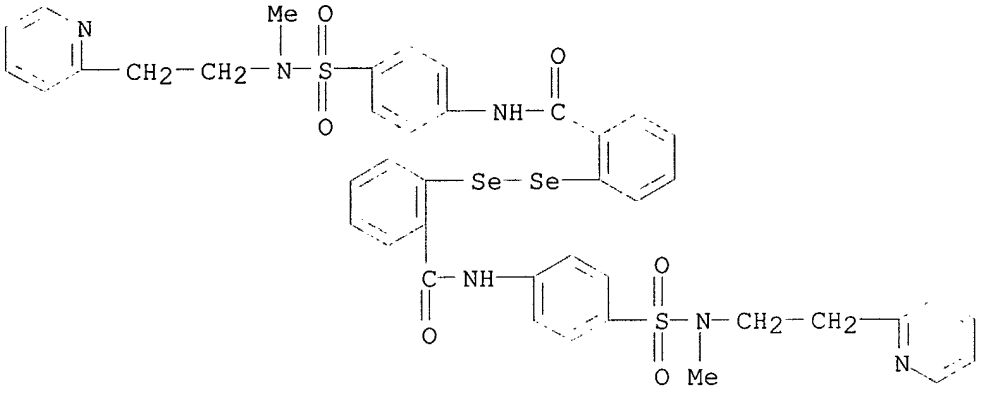
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L35 15 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN **Benzamide, 2,2'-diselenobis[N-[4-[(acetylmethylamino)sulfonyl]phenyl]- (9CI)**
MF **C32 H30 N4 O8 S2 Se2**



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L35 15 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN **Benzamide, 2,2'-diselenobis[N-[4-[[methyl[2-(2-pyridinyl)ethyl]amino]sulfonyl]phenyl]- (9CI)**
MF **C42 H40 N6 O6 S2 Se2**



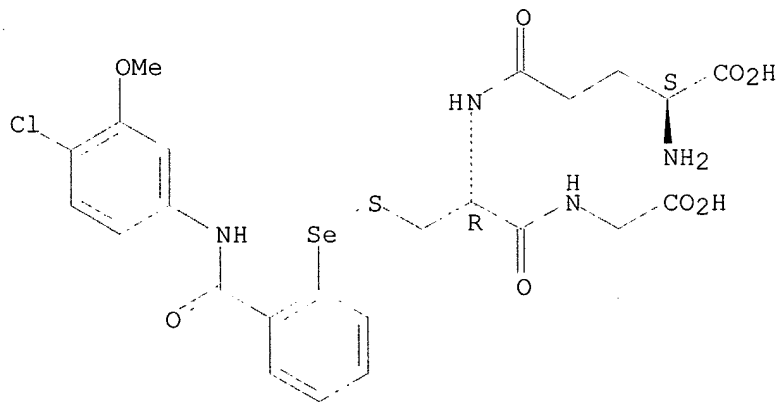
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):end

=> d sca l38

L38 16 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN **Glycine, N-[S-[[2-[[(4-chloro-3-methoxyphenyl)amino]carbonyl]phenyl]seleno]-N-L-.gamma.-glutamyl-L-cysteinyl]- (9CI)**
MF **C24 H27 Cl N4 O8 S Se**

Absolute stereochemistry.

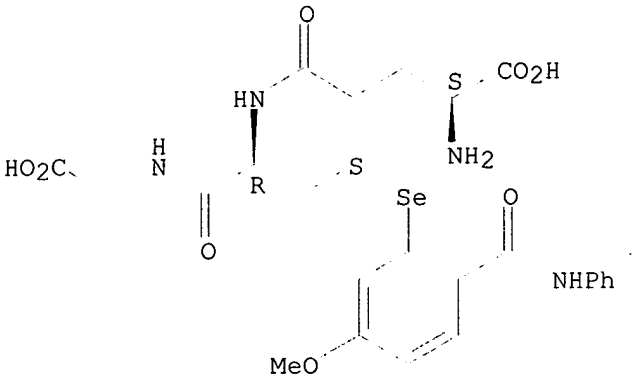


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):5

L38 16 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN **Glycine, N-[N-L-.gamma.-glutamyl-S-[[5-methoxy-2-[(phenylamino)carbonyl]phenyl]seleno]-L-cysteinyl]- (9CI)**
MF **C24 H28 N4 O8 S Se**

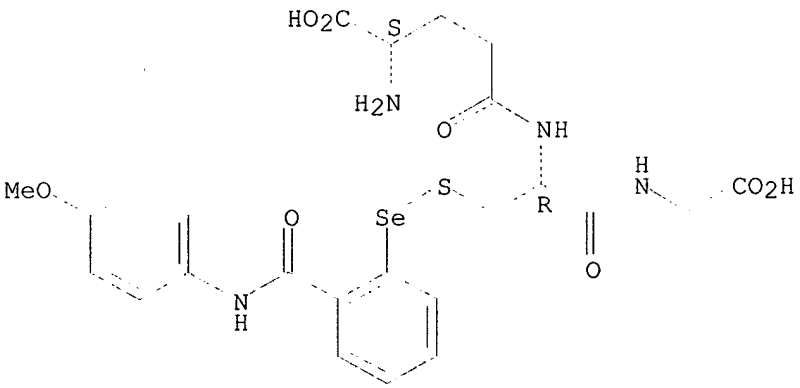
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L38 16 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN **Glycine, N-[N-L-.gamma.-glutamyl-S-[[2-[[(4-methoxyphenyl)amino]carbonyl]phenyl]seleno]-L-cysteinyl]- (9CI)**
MF **C24 H28 N4 O8 S Se**

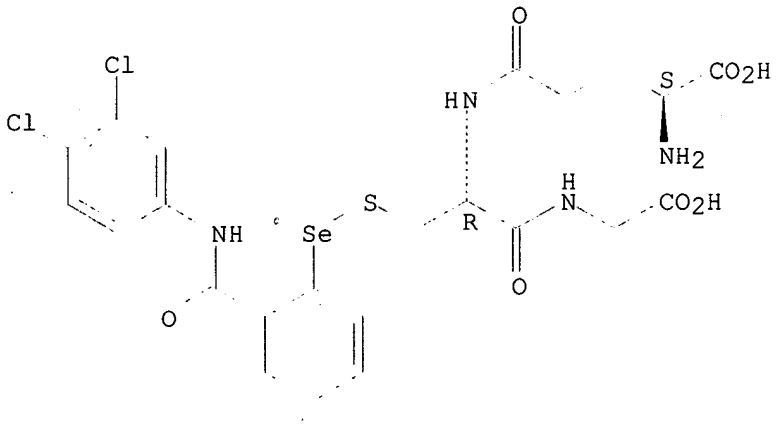
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L38 16 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN **Glycine, N-[S-[[2-[[(3,4-dichlorophenyl)amino]carbonyl]phenyl]seleno]-N-L-.gamma.-glutamyl-L-cysteinyl]- (9CI)**
MF **C23 H24 Cl2 N4 O7 S Se**

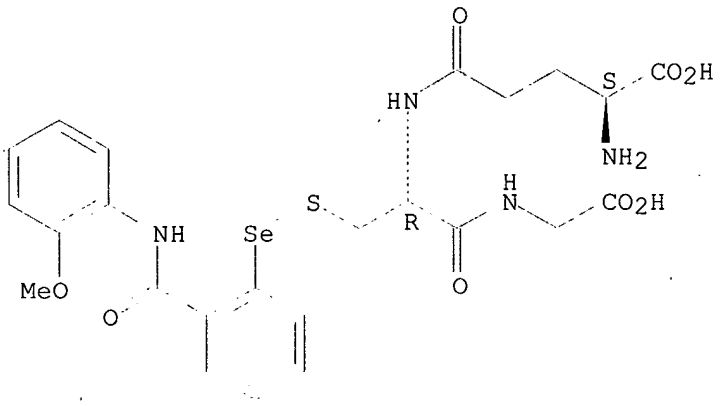
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L38 16 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN **Glycine, N-[N-L-.gamma.-glutamyl-S-[[2-[[(2-methoxyphenyl)amino]carbonyl]phenyl]seleno]-L-cysteinyl]- (9CI)**
MF **C24 H28 N4 O8 S Se**

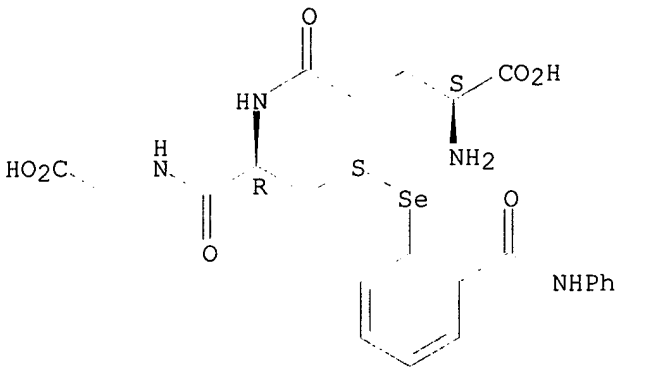
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L38 16 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN **Glycine, L-.gamma.-glutamyl-S-[[2-[(phenylamino)carbonyl]phenyl]seleno]-L-cysteinyl- (9CI)**
MF **C23 H26 N4 O7 S Se**

Absolute stereochemistry.

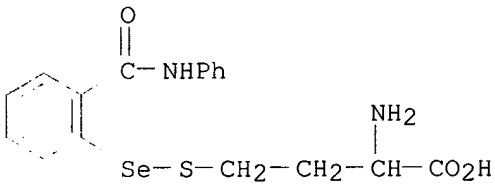


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):end

=> d sca l39

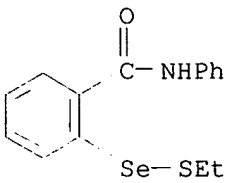
L39 52 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Homocysteine, S-[[2-[(phenylamino)carbonyl]phenyl]seleno]- (9CI)
MF **C17 H18 N2 O3 S Se**



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

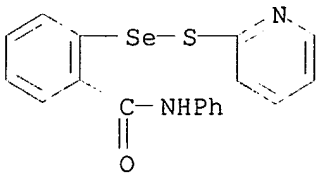
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):10

L39 52 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Ethanesulfenoselenoic acid, 2-[(phenylamino)carbonyl]phenyl ester (9CI)
MF **C15 H15 N O S Se**



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

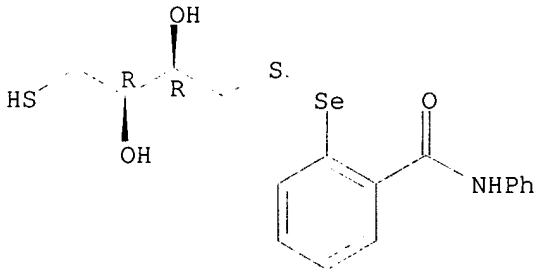
L39 52 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN 2-Pyridinesulfenoselenoic acid, 2-[(phenylamino)carbonyl]phenyl ester (9CI)
MF **C18 H14 N2 O S Se**



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

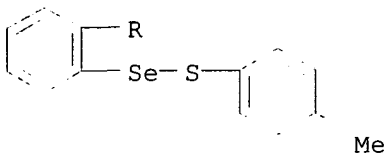
L39 52 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN 1-Butanesulfenoselenoic acid, 2,3-dihydroxy-4-mercapto-, 2-[(phenylamino)carbonyl]phenyl ester, (R*,R*)- (9CI)
MF **C17 H19 N O3 S2 Se**

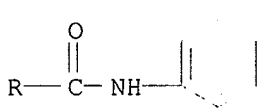
Relative stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

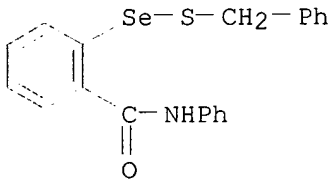
L39 52 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Benzenesulfenoselenoic acid, 4-methyl-, 2-[[(4-methylphenyl)amino]carbonyl]phenyl ester (9CI)
MF **C21 H19 N O S Se**





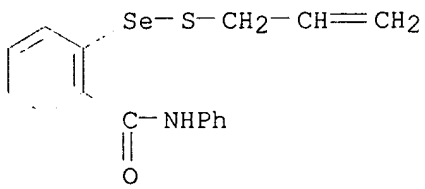
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L39 52 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Benzenemethanesulfenoselenoic acid, 2-[(phenylamino)carbonyl]phenyl ester (9CI)
MF **C20 H17 N O S Se**



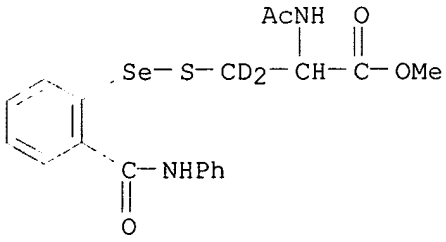
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L39 52 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN 2-Propene-1-sulfenoselenoic acid, 2-[(phenylamino)carbonyl]phenyl ester (9CI)
MF **C16 H15 N O S Se**

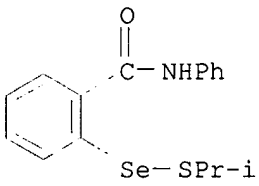


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L39 52 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Cysteine-3,3-d2, N-acetyl-S-[[2-[(phenylamino)carbonyl]phenyl]seleno]-, methyl ester (9CI)
MF **C19 H18 D2 N2 O4 S Se**



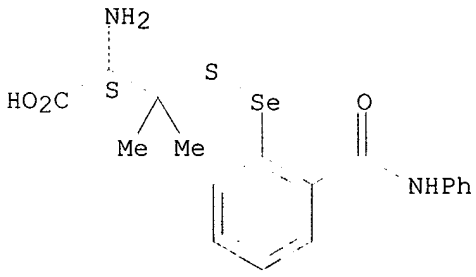
L39 52 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN 2-Propanesulfenoselenoic acid, 2-[(phenylamino)carbonyl]phenyl ester (9CI)
MF **C16 H17 N O S Se**



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L39 52 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN D-Valine, 3-[[[2-[(phenylamino)carbonyl]phenyl]seleno]thio]- (9CI)
MF **C18 H20 N2 O3 S Se**

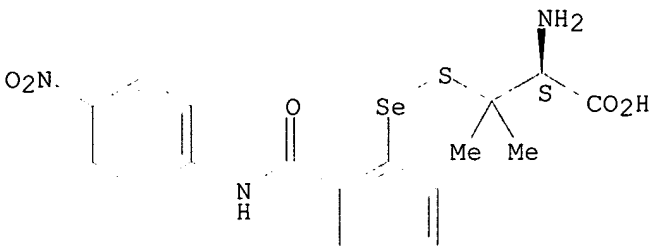
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L39 52 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN D-Valine, 3-[[[2-[[(4-nitrophenyl)amino]carbonyl]phenyl]seleno]thio]- (9CI)
MF **C18 H19 N3 O5 S Se**

Absolute stereochemistry.

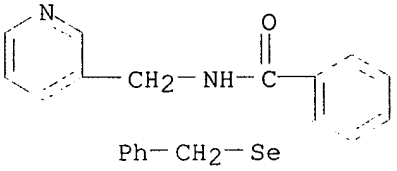


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):end

=> d sca l40

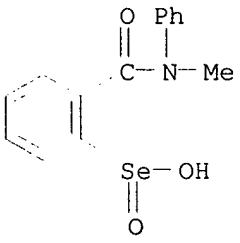
L40 143 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Benzamide, 2-[(phenylmethyl)seleno]-N-(3-pyridinylmethyl)- (9CI)
MF C20 H18 N2 O Se



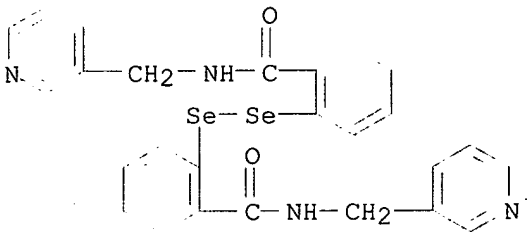
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):5

L40 143 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Benzeneseleninic acid, 2-[(methylphenylamino)carbonyl]- (9CI)
MF C14 H13 N O3 Se

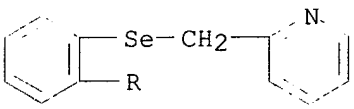


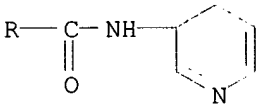
L40 143 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Benzamide, 2,2'-diselenobis[N-(3-pyridinylmethyl)- (9CI)
MF C26 H22 N4 O2 Se2



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

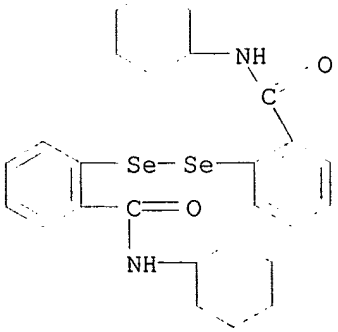
L40 143 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Benzamide, N-3-pyridinyl-2-[(2-pyridinylmethyl)seleno]-, monohydrochloride (9CI)
MF C18 H15 N3 O Se . Cl H





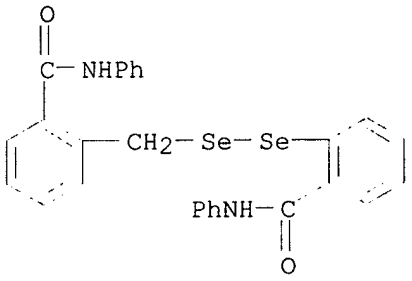
● HCl

L40 143 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Benzamide, 2,2'-diselenobis[N-cyclohexyl- (9CI)
MF C26 H32 N2 O2 Se2



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L40 143 ANSWERS REGISTRY COPYRIGHT 2003 ACS
IN Benzamide, N-phenyl-2-[[[2-[(phenylamino)carbonyl]phenyl]diseleno]methyl]-
(9CI)
MF C27 H22 N2 O2 Se2

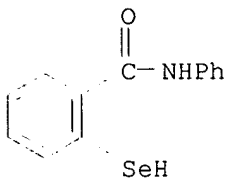


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):end

=> d l51 ide can

L51 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2003 ACS
RN **139015-80-8** REGISTRY
CN Benzamide, N-phenyl-2-selenyl- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN N-Phenyl-2-carboxamidobenzeneselenol
MF C13 H11 N O Se
SR CA
LC STN Files: CA, CAPLUS, MEDLINE, TOXCENTER, USPAT2, USPATFULL



9 REFERENCES IN FILE CA (1962 TO DATE)
2 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
9 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 133:271642

REFERENCE 2: 132:217137

REFERENCE 3: 132:69347

REFERENCE 4: 125:230470

REFERENCE 5: 122:177623

REFERENCE 6: 122:907

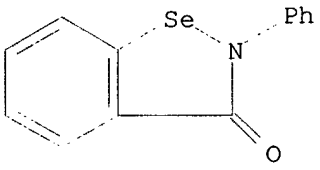
REFERENCE 7: 118:73610

REFERENCE 8: 118:764

REFERENCE 9: 116:143221

=> d l52 ide can

L52 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2003 ACS
RN **60940-34-3** REGISTRY
CN 1,2-Benzisoselenazol-3(2H)-one, 2-phenyl- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN 2-Phenyl-1,2-benzisoselenazol-3(2H)-one
CN 2-Phenyl-1,2-benzoisoselenazol-3(2H)-one
CN Ebselen
CN PZ 51
MF C13 H9 N O Se
LC STN Files: ADISINSIGHT, ADISNEWS, AGRICOLA, BEILSTEIN*, BIOBUSINESS, BIOSIS, BIOTECHNO, CA, CANCERLIT, CAPLUS, CASREACT, CEN, CHEMCATS, CHEMINFORMRX, CIN, CSCHEM, DDFU, DRUGNL, DRUGU, DRUGUPDATES, EMBASE, IPA, MEDLINE, MRCK*, PHAR, PROMT, RTECS*, SYNTHLINE, TOXCENTER, USAN, USPAT2, USPATFULL
(*File contains numerically searchable property data)
Other Sources: WHO



413 REFERENCES IN FILE CA (1962 TO DATE)
19 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
415 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 138:84749

REFERENCE 2: 138:83310

REFERENCE 3: 138:68712

REFERENCE 4: 138:33174

REFERENCE 5: 138:11174

REFERENCE 6: 137:370035

REFERENCE 7: 137:365444

REFERENCE 8: 137:350476

REFERENCE 9: 137:346030

REFERENCE 10: 137:329273